

The Calculation of Molecular Opacities

Richard Freedman

The theoretical modeling of the properties and emergent spectra of extra solar giant planets and brown dwarfs requires an accurate and detailed knowledge of the sources of molecular opacity in these objects. In the past few years, many new extra solar planets and brown dwarfs have been discovered using new observational techniques and better, larger telescopes. In order to better understand the physical properties of these new objects and to relate their properties to the properties of other solar systems, astronomers have been using computer-generated models to reproduce their observed properties. This scenario allows a direct comparison between theory and observations and helps to constrain physical properties such as mass, radius, and chemical composition. These objects span the range between the gas giants of our own solar system (Jupiter) and objects almost large enough to burn hydrogen in their interior and thus become stars (brown dwarfs). An accurate theoretical model requires a thorough knowledge of the molecular opacities of a large number of different species, because the temperature in the atmospheres of these objects spans a range from 100 kelvin up to several thousand degrees. Because of the wide range of physical conditions encountered, modelers need molecular opacities up to a range of temperatures that go far beyond the normal range of molecular data from laboratory studies. The purpose of this research is to extend the range of available molecular opacities up to the higher temperatures needed by the modelers.

This extension has been accomplished by using a combination of theoretical techniques combined with available observational data to predict lines of various molecules such as CH₄, VO, and CrH. As an example of what has been accomplished, consider the cases of CH₄, H₂O, and TiO: (methane, water, and titanium oxide). The list of spectral lines was extended for all these species to include lines that will become important at higher temperatures, even though these lines are practically unobservable at room temperatures. Water and methane, in particular, are very important sources of opacity in these objects, and the inclusion of adequate opacity is very

important to properly evaluate their spectra and construct physically realistic models.

In doing this work, the researcher made use of the work of other Ames researchers, especially the work of David Schwenke of the Computational Chemistry Branch. Comparison with observations shows that more work remains to be done to provide opacities that are physically realistic at the highest temperatures, especially for methane and (less so for) water. Even so, the latest models for objects such as the brown dwarf Gl229B (Gliese 229B) show good agreement with the best available observations.

Point of Contact: R. Freedman
(650) 604-0316
freedman@darkstar.arc.nasa.gov

Mars Atmosphere and Climate

Jeffery L. Hollingsworth, Robert M. Haberle, James Schaeffer

Furthering our understanding of the global atmospheric circulation on Mars is the focus of this research at Ames Research Center. As in Earth's atmosphere, Mars' atmospheric circulation exhibits variability over a vast range of spatial and temporal scales. Some of these processes are driven by similar physical processes (for example, Hadley circulation cells; global-scale thermal tidal modes; planetary waves forced via flow over large-scale orographic complexes like Earth's Himalayan plateau; and developing, traveling, and decaying extratropical weather cyclones associated with pole-to-equator thermal contrasts). Other sources of variability arise from distinctly Martian physical mechanisms (for example, condensation (sublimation) during the winter (summer) season of the primary chemical constituent of the atmosphere (predominantly carbon dioxide (CO₂), and regional- and global-scale dust storms). Ultimately, these investigations aspire to improve our knowledge of the dynamics of the planet's present environment and past climates, and from a comparative planetology perspective, to better

understand similar processes that govern the dynamics of the Earth's climate.

In this endeavor, the primary tool used is the Ames Mars General Circulation Model (MGCM). The MGCM is a time-dependent, three-dimensional, numerical model of the hydrodynamic state of the atmosphere as determined by self-consistent algorithms for radiative (for example, solar and infrared absorption, emission and scattering in the planet's tenuous and frequently dust-laden atmosphere) and near-surface processes (for example, a boundary-layer dissipation associated with atmospheric turbulence). In parallel efforts, spacecraft data from the recent Mars Pathfinder mission and the ongoing Mars Global Surveyor (MGS) mission are utilized to validate the climate-simulation results, while at the same time both mechanistic and full-up MGCM simulations can offer a global context for the remotely sensed data.

Investigation of the middle- and high-latitude meteorological environment using a very-high-resolution version of the MGCM has recently been conducted. This research is motivated by Hubble Space Telescope (HST) observations of "comma"-shaped cloud formations and large-scale dust activity in the polar region during early northern spring and summer, and by MGS Mars Observer Camera (MOC) imaging of condensate cloud structures in the polar environment during this season. Modeling at high spatial resolution is necessary in order to illuminate processes important to local and regional dust activity, as well as condensate cloud formation, structure, and evolution within the edge of Mars' seasonal polar caps. It has been found that near-surface and upper-level fronts (that is, narrow zones with enhanced mass density, momentum, and thermal contrasts within individual extratropical cyclones) can form in Mars' intense high-latitude baroclinic zone, and the associated frontal circulations are sufficient to raise dust in high latitudes.

Shown in figure 1 in a spherical projection view are examples of these results for simulations that include recent MGS Mars Observer Laser Altimeter (MOLA) topography in the climate model. Solid contours correspond to potential temperature and arrows correspond to the instantaneous horizontal wind. Near the prime meridian (center longitude of each panel), a clear rarefaction, stretching and deformation of the temperature field, can be seen. This rarefaction is caused by intense local circulations associated with traveling weather systems in middle latitudes (that is, transient baroclinic eddies). These systems are Mars analogs of traveling high- and low-pressure systems that occur in Earth's extratropics associated with instability of the tropospheric jet stream. Note the profound sharpness of the frontal systems, as well as their vast north-south (that is, meridional) scale. The weather fronts appear to be favorably triggered near the high-relief regions of the western hemisphere and subsequently intensify rapidly in the low-relief areas to the east. Based on low-horizontal-resolution modeling of Mars' transient baroclinic waves, the latter geographic region corresponds to a preferred region for cyclone development (that is, a "storm zone").

Both the data analysis and modeling efforts can significantly enhance the assessment of Mars' present climate, and thereby provide a more comprehensive climate database for future missions scheduled during the Mars Surveyor program.

Point of Contact: J. Hollingsworth
(650) 604-6275
jeffh@humbabe.arc.nasa.gov

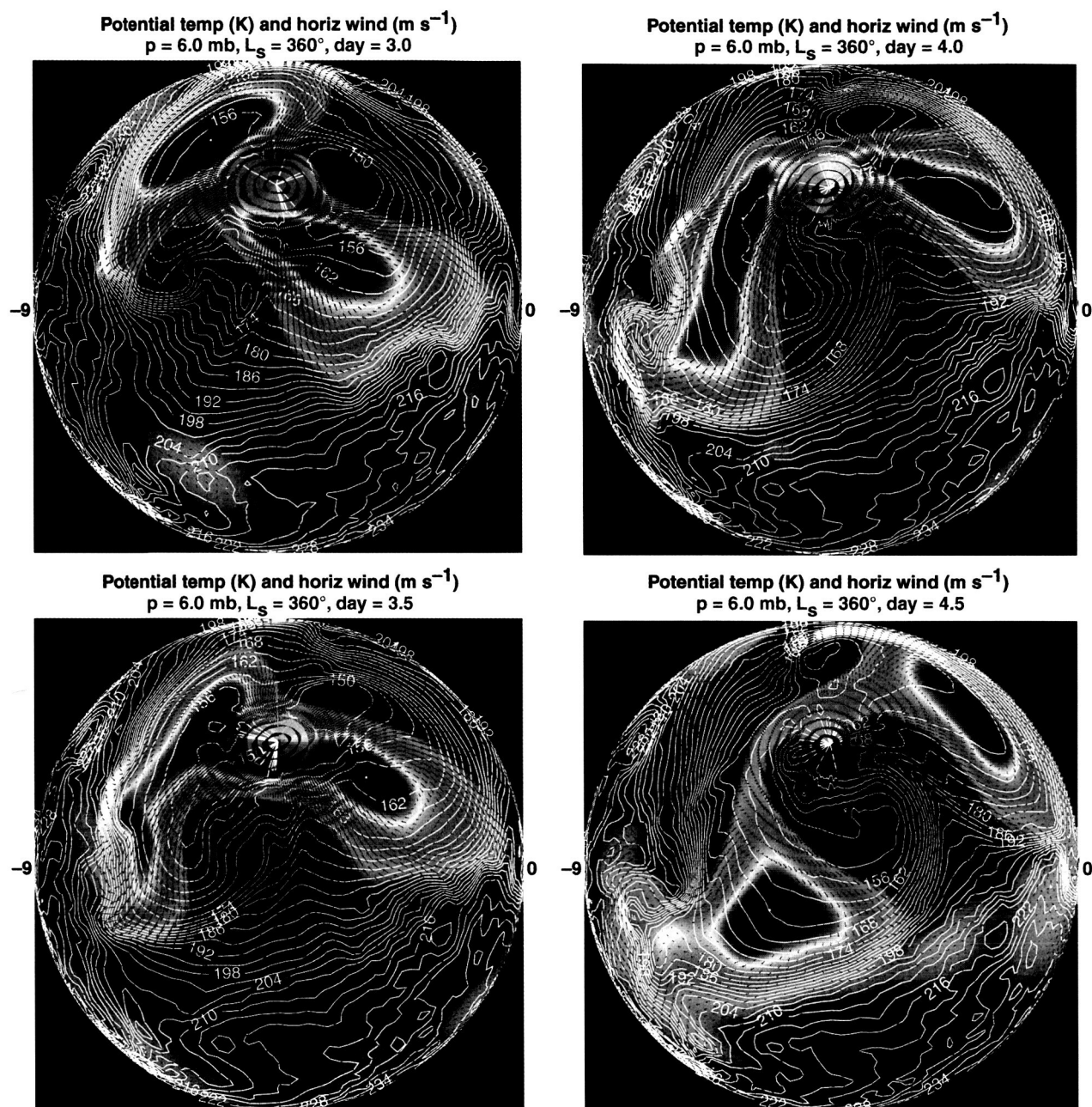


Fig. 1. Potential temperature (kelvin) and horizontal wind (meters per second) at the 6-millibar surface, and instantaneous surface pressure anomaly (color) on (a) day 3.0, (b) day 3.5, (c) day 4.0, and (d) day 4.5, in a MGCM numerical experiment using MGS/MOLA topography. High (anticyclonic) pressure anomaly is red and low (cyclonic) pressure anomaly is black/purple. The temperature contour interval is 3 kelvin.